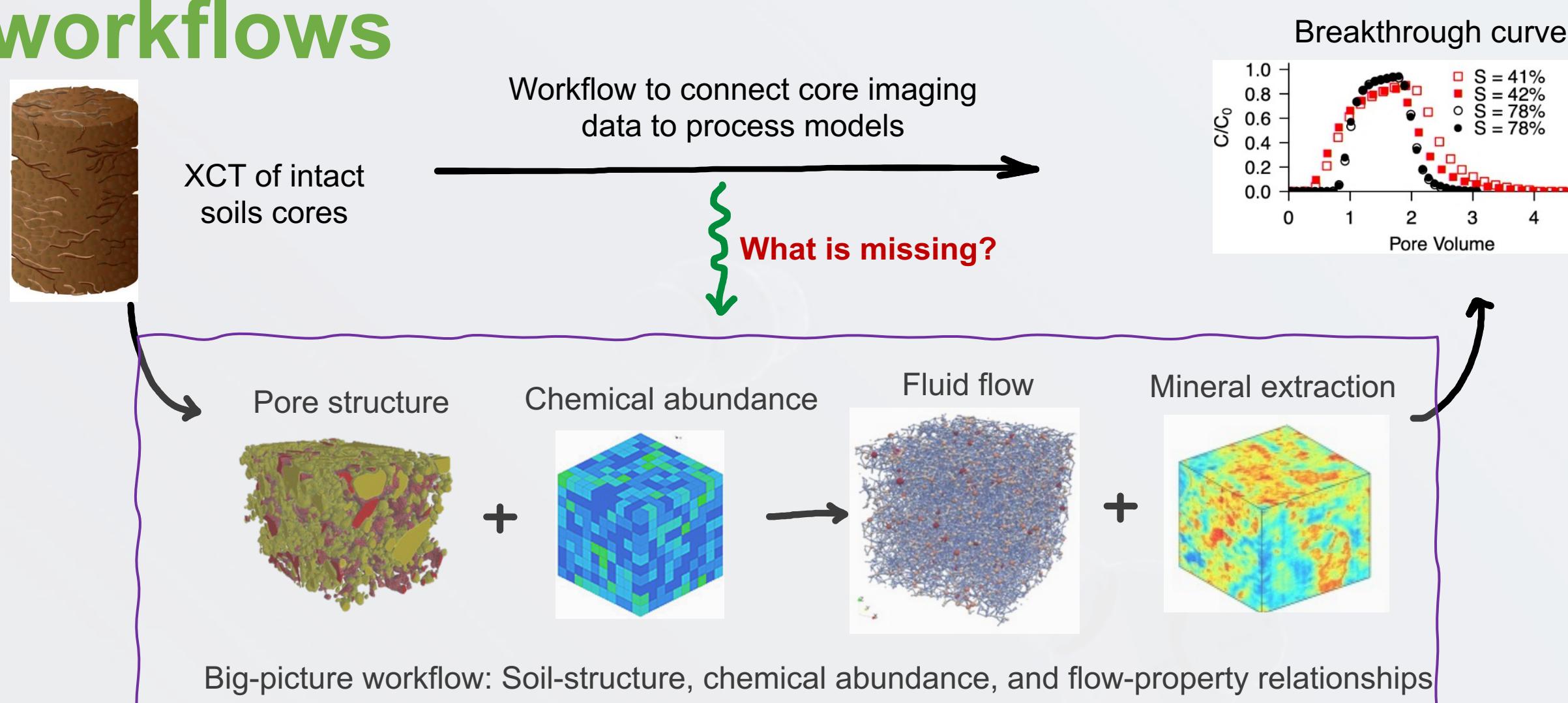


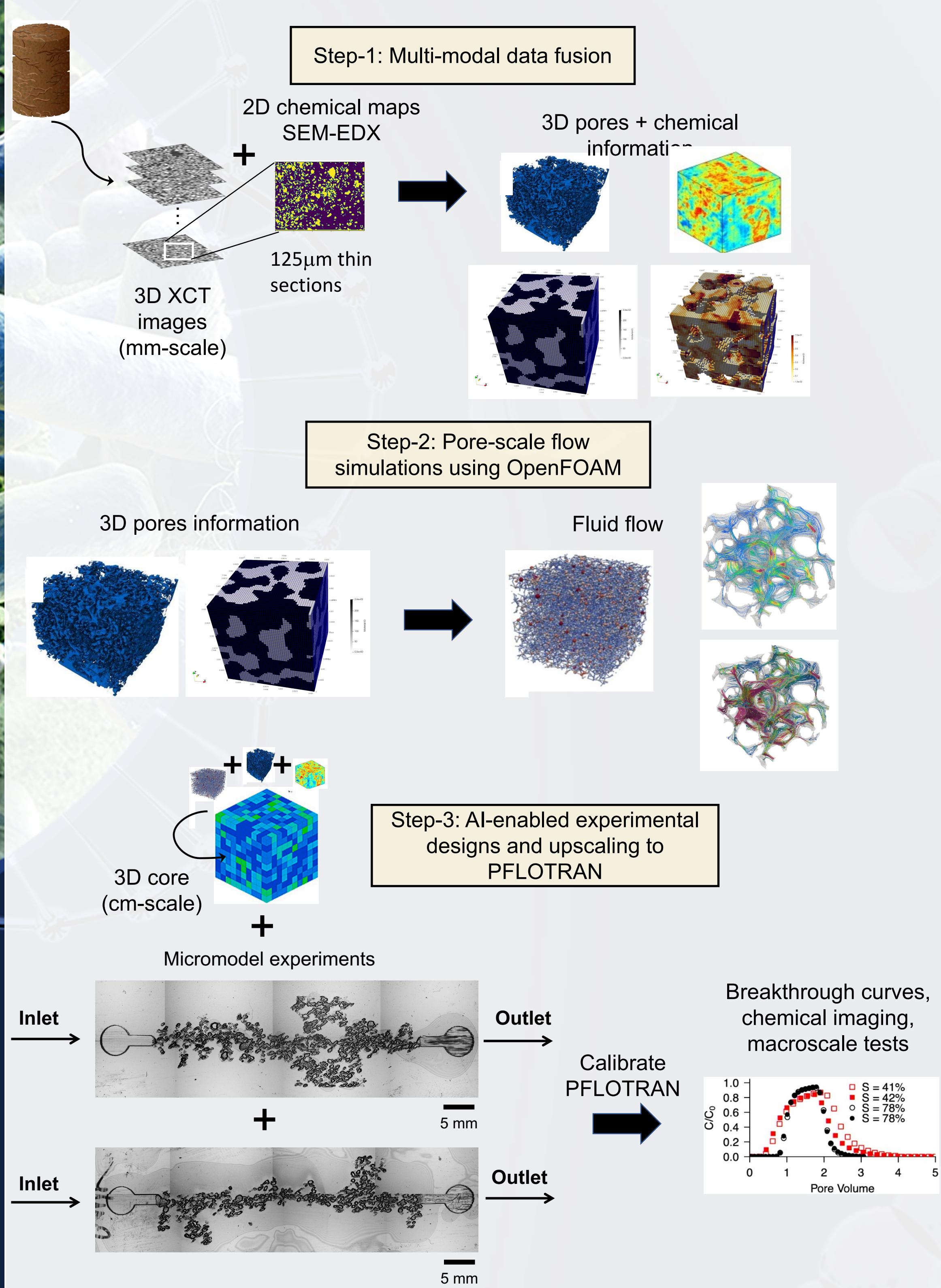
# SoilTwin: Linking experiments and process models using AI/ML by generating reduced complexity digital twins of porous media

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## Importance of SoilTwin: EMSL users are interested in AI-enabled experimental designs and open-source modeling workflows



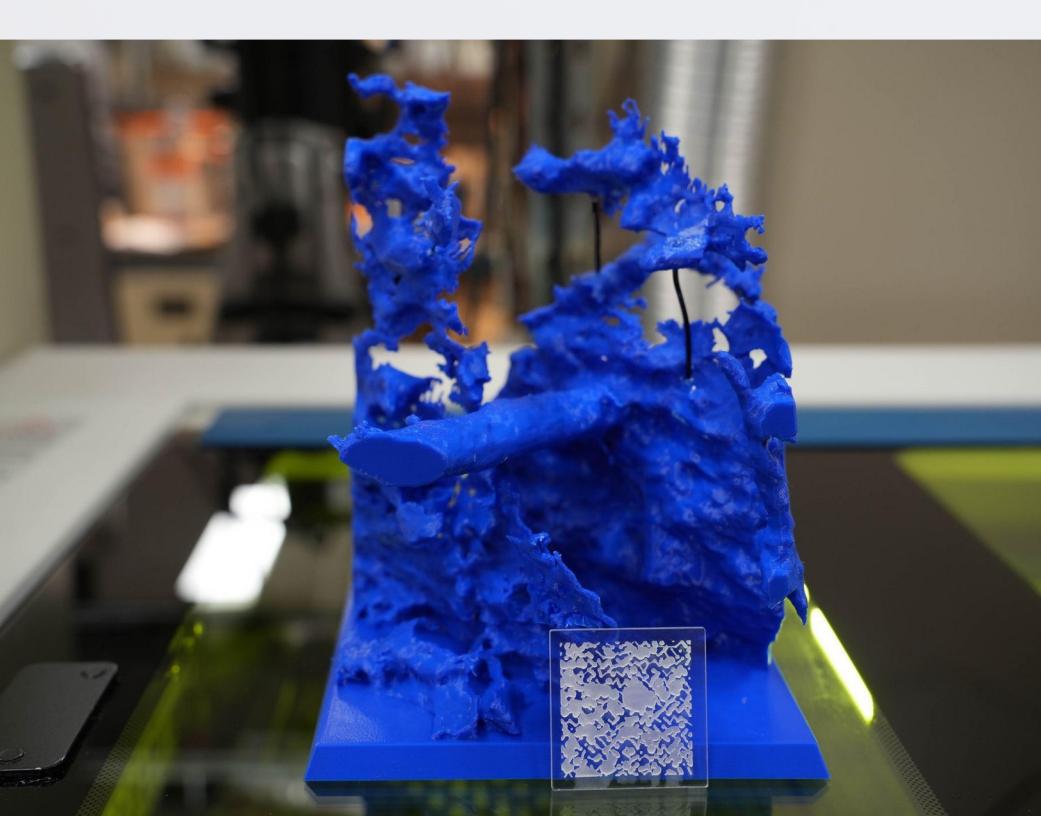
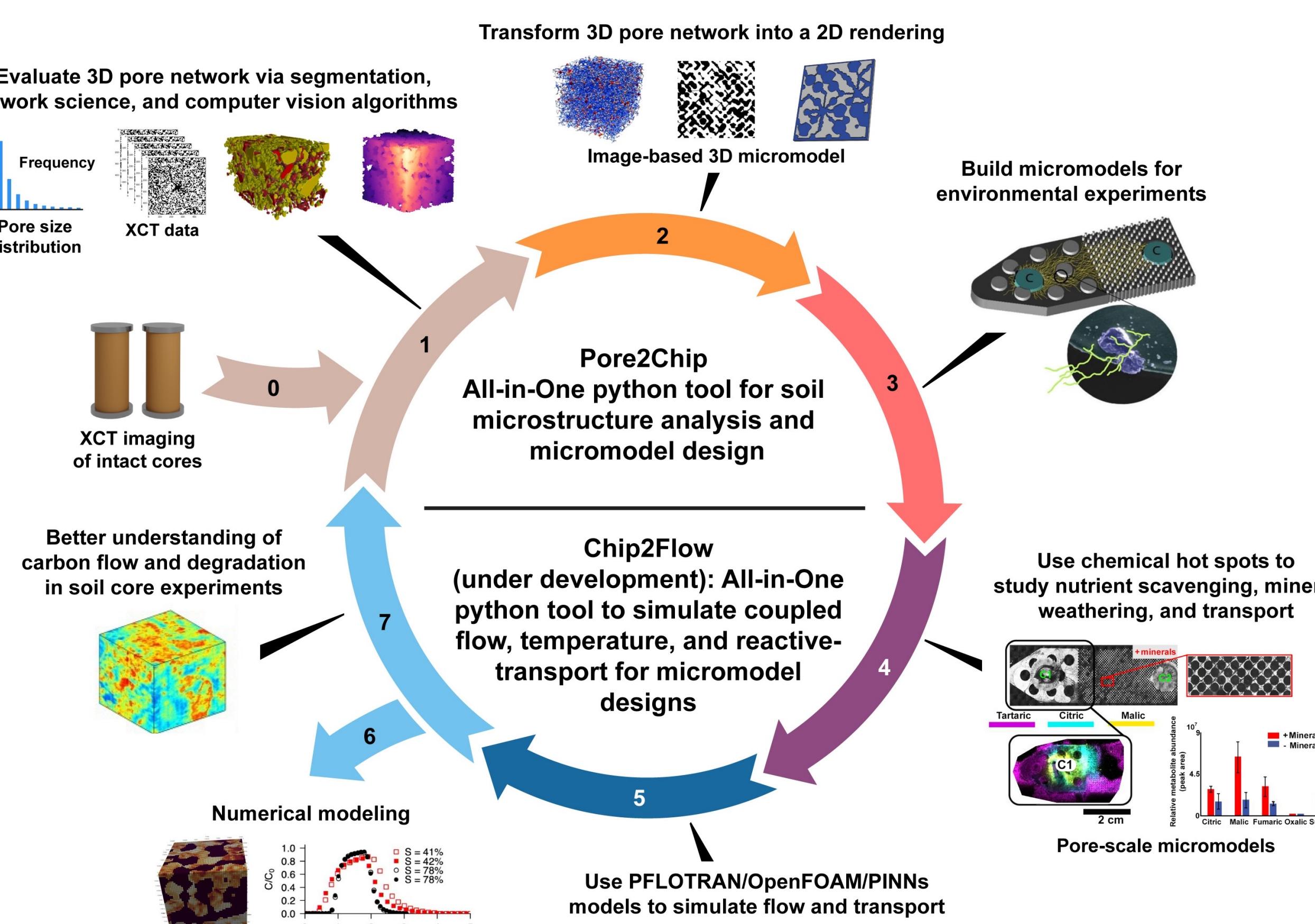
## Key takeaway on structure-flow-chemical property relationships: XCT and SEM-EDX provide detailed information on pore structure and mineral distribution



## SoilTwin: AI-enabled digital twin for porous materials

- SoilTwin has two set of workflows: (1) **Pore2Chip** and (2) **Chip2Flow**
- The **Pore2Chip workflow** is an open-source software that characterizes the pore network of 3-D image files and generates a 2-D representative pore network.
  - Available to user community via EMSL-Computing GitHub and Tahoma:
  - <https://github.com/EMSL-Computing/Pore2Chip>
- The **Chip2Flow workflow** is currently under development, which focuses on pore-scale and upscaling. Emphasis is on coupled flow and reactive-transport with applications to critical minerals and materials (CMM).
  - Will be available to user community via EMSL-Computing GitHub and Tahoma:
  - <https://github.com/EMSL-Computing/Chip2Flow>
- **Fabrication:** EMSL has many different additive manufacturing fabrication capabilities for Pore2Chip, which includes laser etching or photolithography.
- These lab-on-chip micromodels are compatible with existing EMSL characterization technologies such as in situ mass spectrometry imaging.

### Lab-on-chip designs to accelerate model-data-experiment loop informed by MONet datasets

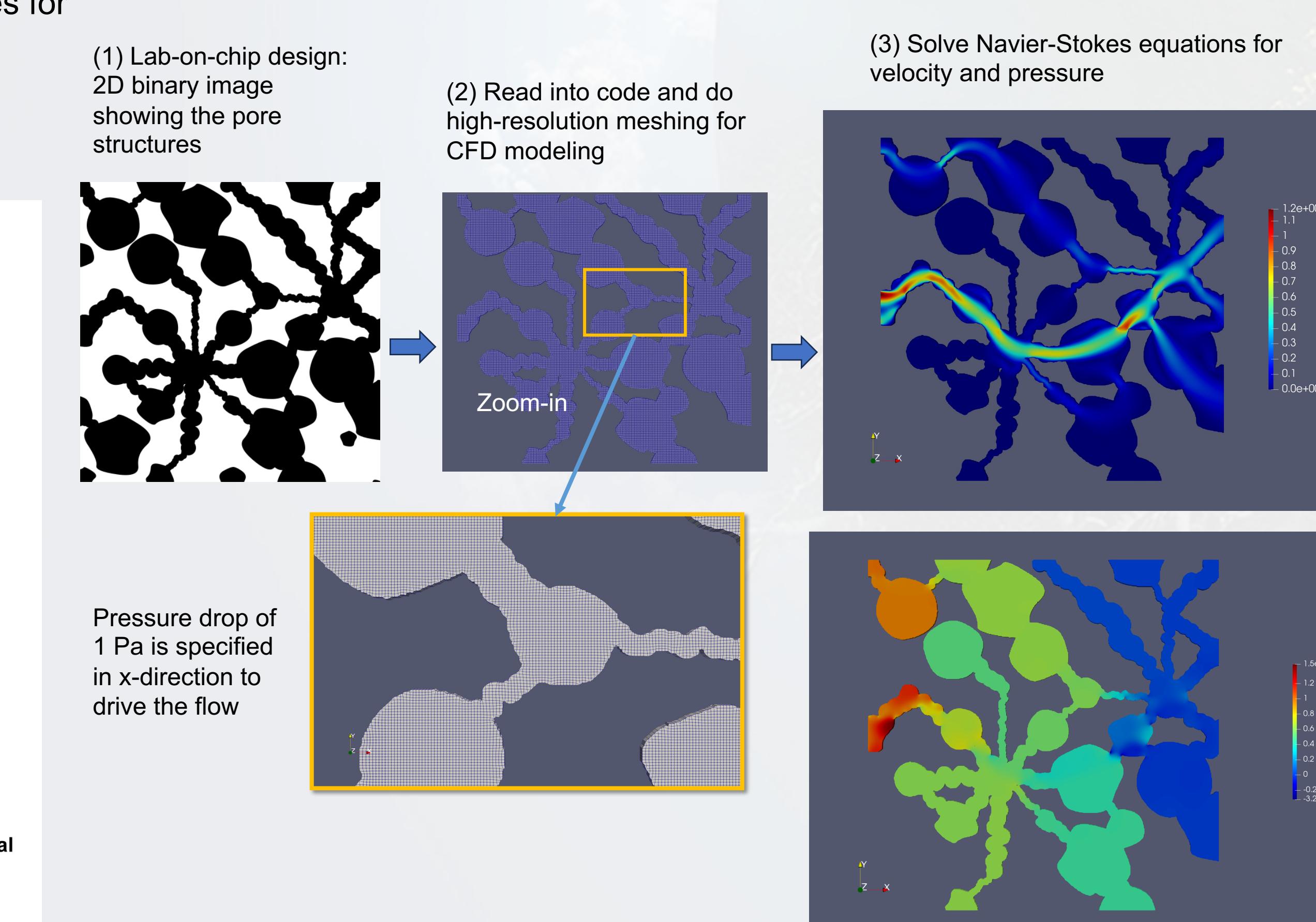


**Key takeaway on pore-scale modeling:** Spatial heterogeneity of the pore-structure directly impacts the velocity field, pressure distribution, and mineral recovery

### Pore2Chip models (under development)



### Chip2Flow models (under development)



## Timeliness, user impact, and next steps

SoilTwin is being extended to critical mineral and materials applications:

- We can test treatments that might liberate them from certain mineral composites, test microbial sequestration/liberation/processing, all with control of some key soil microstructure properties.
- Pore2Chip has a lot of user and download traffic. Current there are more than 5000 downloads since its release in July-2024.
- More than 12 different EMSL users (within and outside U.S.) are using various parts of this workflow in their research.

